<u>Amendments to the Claims</u>

Claim 1 (currently amended): A computer-aided method for the provision, identification and description of molecules exhibiting a desired activity comprising;

a molecular modeling step in which molecular descriptors are <u>selected</u> ~~determined~~ computationally;

a step of building a combinatorial library of molecules;

a step of selecting candidate molecules which potentially exhibit said desired activity;

a filtering step whereby candidate molecules are filtered using at least one static filter representing a plurality of said molecular descriptors;

a further filtering step whereby candidate molecules are filtered using at least one dynamic filter representing constraints of conformational variations which each candidate molecule must satisfy in order to exhibit said desired activity.

Claim 2 (cancelled)

Claim 3 (withdrawn)

Claim 4 (previously amended): A computer-aided method according to Claim 1 further comprising the step of screening the candidate molecules on the basis of the degree of enrichment provided by each candidate molecule to molecular descriptors.

Claim 5 (previously amended): A computer-aided method according to Claim 1 further comprising the step of deriving one or more criteria associating descriptor values with activity, said criteria including at least one static criterion and at least one dynamic criterion wherein at least one of said criteria is based on a non-linear function of a descriptor value.

-2-

Claim 6 (withdrawn)

Claim 7 (withdrawn)

Claim 8 (previously amended): A computer-aided method
according to Claim 1 further comprising the step of deriving
one or more criteria associating descriptor values with
activity, said criteria including at least one static
criterion and at least one dynamic criterion wherein at least
one of said dynamic criteria is based on the conformational
spaces of a candidate molecule.

Claim 9 (previously amended): A computer-aided method
according to Claim 5 or Claim 8 wherein at least one of said
dynamic criteria is based on a shape descriptor derived from a
3 D autocorrelation vector (3D-ACV) of the candidate molecule.

Claim 10 (previously amended): A computer-aided method
according to Claim 9 wherein the static criteria are
based on physiochemical and topological descriptors at least
some of which are chosen from the following descriptors: Molar
Mass; Ellipsiodal Volume; Molecular Volume; Molar
Refractivity; Lipophilia (LogP); Kappa 1; Kappa 2; Kappa 3;
Kappa Alpha 1; Kappa Alpha 2; Kappa Alpha 3; Flexibility; Kier
Chi V4; Randic Index; Balaban Index; Weiner Index; Sum of
Condition E; Dipolar Moment; Number of C Atoms; Number of O
Atoms; Number of N Atoms; Number of H Atoms; Total Number of
Atoms; Number of Methyl Groups; Number of Ethyl Groups; Number
of Amino Groups; Number of Hydroxyl Groups.

Claims 11-17 (withdrawn)

Claim 18 (currently amended): A computer-aided method for the
provision, identification and description of molecules
exhibiting immunomodulatory activity comprising;

-3-

a step of molecular modeling in which molecular descriptors of a molecule having immunomodulatory activity are selected ~~determined~~ computationally;

a step of building a combinatorial library including molecules having said immunomodulatory activity;

a step of selecting candidate molecules which are potentially immunomodulatory;

a filtering step whereby candidate molecules are filtered using at least one static filter representing a plurality of said molecular descriptors; and

a further filtering step whereby candidate molecules are filtered using at least one dynamic filter representing constraints of conformational variations which each candidate molecule must satisfy in order to exhibit said immunomodulatory activity.

Claim 19 (original): A computer-aided method according to claim 1 wherein the combinatorial library building step comprises building a combinatorial peptide library.

Claim 20 (original): A computer-aided method according to claim 1 wherein the combinatorial library building step comprises building a combinatorial peptoid library.

Claims 21-68 (withdrawn)

Claim 69 (cancelled)

Claims 70-72 (withdrawn)

Claim 73 (previously added): A computer-aided method according to Claim 5 wherein the static criteria are based on physiochemical and topological descriptors at least some of which are chosen from the following descriptors: Molar Mass; Ellipsiodal Volume; Molecular Volume; Molar Refractivity;

-4-

Lipophilia (LogP); Kappa 1; Kappa 2; Kappa 3; Kappa Alpha 1; Kappa Alpha 2; Kappa Alpha 3; Flexibility; Kier Chi V4; Randic Index; Balaban Index; Weiner Index; Sum of Condition E; Dipolar Moment; Number of C Atoms; Number of O Atoms; Number of N Atoms; Number of H Atoms; Total Number of Atoms; Number of Methyl Groups; Number of Ethyl Groups; Number of Amino Groups; Number of Hydroxyl Groups.